

The Least-Action Principle: Theory of Cosmological Solutions and the Radial-Velocity Action

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ABSTRACT

Formulating the equations of motion for cosmological bodies (such as galaxies) in an integral, rather than differential, form has several advantages. Using an integral the mathematical instability at early times is avoided and the boundary conditions of the integral correspond closely with available data. Here it is shown that such a least-action calculation for a number of bodies interacting by gravity has a finite number of solutions, possibly only one. Characteristics of the different possible solutions are explored. The results are extended to cover the motion of a continuous fluid. A method to generalize an action to use velocities, instead of positions, in boundary conditions, is given, which reduces in particular cases to those given by Giavalisco et al. (1993) and Schmoldt & Saha (1998) . The velocity boundary condition is shown to have no effect on the number of solutions.

Subject headings: cosmology:theory—galaxies: kinematics and dynamics—galaxies: formation—methods: numerical

1. Introduction

The present motions of cosmological objects, in particular galaxies, are functions of their past history. In principle one might discover the shape of the past by calculating presently observed positions and motions backward. However, in doing this we are faced immediately with two problems. First, their velocities in the plane of the sky are not known, and their distances not known accurately; so perhaps half the information needed to start the calculation by Newton's equations is there. Second, if the trajectories of the galaxies are to be traced back to very early times distances become very small and corresponding gravitational forces very large. Small errors in present velocities or positions become heavily magnified, resulting in galaxies being formed at infinite speeds. The problem is mathematically unstable, rather like trying to roll a marble to the top of a glass mountain, and requiring that it stop exactly on the summit¹.

To avoid these difficulties Peebles (1989, 1990, 1994) formulated the problem in integral rather than differential form. This traded the relative simplicity and definiteness of differential equations for the stability of the integral. The most important consideration in moving from the differential to integral form of the problem (apart from the mechanics of implementation) is the fact that, with the same boundary conditions, an integral calculation may produce several (or many) solutions. An obvious question to answer is just how many there are. This is something more than a purely mathematical concern. Of course, if the numerical calculation of solutions can be guided in some way there is the potential for a large savings in computer time, and if the number of solutions is limited the search may be stopped when all are found. Conversely, if the number of solutions is very large or infinite, the usefulness of the calculation is thrown into doubt (unless some method of selecting more probable solutions is found). But the question is more fundamental than that, for the variational formulation of the cosmological problem corresponds closely to the limits of our knowledge. When the present radial velocities and positions on the sky of a number of bodies are specified and the Big Bang postulated, we find the end conditions are fixed; the action is determined by relevant physics. The mathematical question is thus transformed into a cosmological one.

The subject of this study is the mathematical theory of variational calculations as applied to the cosmological problem. That problem is defined as the determination of the motion of a number of bodies moving under gravitational interaction, with the requirement that all bodies must be at the same point (in proper coordinates) at $t = 0$.

¹Valtonen et al. (1993) have found some possible solutions for the motion of the major galaxies in the Local Group and the Maffei 1/IC 342 Group by integrating equations of motion forward from an early time. However, it is not clear that this method is generally applicable, and in any case requires a great deal of hunting about in parameter space; for their result, the Valtonen group integrated ten thousand situations.

Newtonian, rather than relativistic, calculations are employed throughout².

The cosmological problem may be interpreted as a rough approximation of the motion of galaxies, each galaxy simulated by a point mass interacting only through gravity. This is the way most least-action calculations have proceeded, and is not a bad approximation considering the uncertainties in such data as distances and masses. It would be more accurate, however, to consider the objects to represent the dark matter halos of galaxies (which as far as is known interact *only* through gravity). The point-mass approximation provides a reasonable simulation of gravitational effects, since multipole moments decay rapidly with distance (Dunn & Laflamme 1995 found them to be quite unimportant), and in any case the conclusions of this study are not affected by the detailed form of the gravitational potential used.

Of course, identifying whole galaxies with single bodies ignores internal structure (which may be significant in some cases) and the effects of mergers (which certainly are significant); Dunn & Laflamme (1995) found some additional problems. To address these matters one must turn to a continuous fluid formulation of the problem. Section 6 generalizes the discrete-body results to this more complicated situation.

2. The First Variation

Consider first the problem of minimizing the integral

$$I = \int_{t_0}^{t_1} (T - V) dt = \int_{t_0}^{t_1} L(q_i, \dot{q}_i, t) dt \quad (1)$$

where the kinetic energy T is quadratic in the generalized velocities \dot{q}_i (or, alternatively, in the generalized momenta $\partial L / \partial \dot{q}_i = p_i$) and the potential V does not depend on velocity. The end points $q_i(t_0)$ and $q_i(t_1)$ are given. (This is interpreted dynamically by constructing a path $\mathbf{r}(t)$ in $3n$ -dimensional space using the vectors $\mathbf{r}_j(q_i(t))$, $j = 1$ to n , $i = 1$ to $3n$, where the \mathbf{r}_j are the paths of the n bodies in 3-dimensional space.) For small variations the change in the action is given by a truncated expansion in a Taylor's series (treating q_i, \dot{q}_i as independent variables):

$$\delta \int_{t_0}^{t_1} L(q_i, \dot{q}_i, t) dt = \int_{t_0}^{t_1} \sum_i \left[\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right] dt = 0. \quad (2)$$

Equation (2) can be integrated by parts to give

$$\int_{t_0}^{t_1} \sum_i \left[\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \right] \delta q_i dt + \sum_i \left[\frac{\partial L}{\partial \dot{q}_i} \delta q_i \right]_{t_0}^{t_1} = 0 \quad (3)$$

²See Peebles (1980) and Bondi (1960) for the validity of this approach.

and if the variation in \mathbf{r} vanishes at the end points (that is, if the end points are fixed) the boundary term is zero. The requirement that the integral vanish for arbitrary variations $\delta\mathbf{r}$ results in the Euler-Lagrange equations:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = 0. \quad (4)$$

These are the dynamic equations, identical with those derived from (for example) forces and accelerations. The correspondence between the dynamic equations and the vanishing of the first variation of equation (1) is *Hamilton's Principle*.

A path which minimizes the integral will thus always satisfy the dynamic equations. However, the converse is not necessarily true: a path satisfying the Euler-Lagrange equations is not guaranteed to provide a minimum of the corresponding integral. For sufficiently small path lengths a minimum does result (see, for example, Whittaker 1959, pp. 250-2); beyond a certain point the path will make the integral stationary, but not necessarily a minimum. Finding the point that determines the limit of application of the least-action technique (strictly interpreted) to the dynamical problem will be discussed below³.

Adding a total derivative (in multiple dimensions, a divergence expression) will not change the Euler-Lagrange equations (see Courant and Hilbert 1953, p. 296) but can change the boundary terms. For instance, varying

$$\int_{t_0}^{t_1} \left[L - \sum_j \frac{d}{dt} \left(q_j \frac{\partial L}{\partial \dot{q}_j} \right) \right] dt \quad (5)$$

leads to

$$\int_{t_0}^{t_1} \sum_j \left[\frac{\partial L}{\partial q_j} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) \right] \delta q_j dt - \sum_j \left[q_j \delta \left(\frac{\partial L}{\partial \dot{q}_j} \right) \right]_{t_0}^{t_1} = 0. \quad (6)$$

If the original Lagrangian is quadratic in \dot{q}_j , recovery of the Euler-Lagrange equations requires that either $q_j = 0$ or $\delta \dot{q}_j = 0$ in each boundary term. In the second case, it is the velocity at the end point which is the fixed boundary condition, rather than the position. This raises the possibility of using a radial velocity, rather than a distance, as the end point in a cosmological calculation. In fact Giavalisco et al. (1993) have considered such a mixed boundary condition, in one place using it to modify a set of approximating functions and in another expressing it as a canonical transformation of variables. Their approaches are in practice equivalent to this one. Schmoldt & Saha (1998) have succeeded in using a velocity endpoint in their numerical calculation.

It is straightforward to show that the boundary term added here does not change Whittaker's conclusion above. Note that the coordinates q_j which provide velocity

³Whittaker calls Euler's Principle, which appears later, the *Least Action* Principle; however, Hamilton's Principle has also been called this. To distinguish between the two I will use the names of the mathematicians and call them collectively Least Action Principles.

boundary conditions may be all or only some of the total number of coordinates q_i , as long as the total derivative is adjusted accordingly.

2.1. Variable Endpoints

If the radial velocity is to be used as a form of endpoint, rather than the (less accurately known) radial distance, the theory of “free” endpoints (constrained to move on a manifold of some description) comes into play. In addition to the Euler-Lagrange equations, the solution must now satisfy the *transversality condition* which results from the minimization of the variation at a free end point⁴. As expressed in Morse’s (1934) notation, this condition is

$$\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) dt^s + \sum_i \frac{\partial L}{\partial \dot{q}_i} dq_i^s = 0 \quad (7)$$

where the superscript s denotes a differential taken along the end manifold (s takes on values designating the initial or final end points) and L is the integrand.

Applied to the Lagrangian for a number of bodies moving under their mutual gravity

$$L = \sum_i m_i \left(\frac{1}{2} (\dot{r}_i^2 + r_i^2 \dot{\theta}_i^2 + r_i^2 \sin^2 \theta_i \dot{\phi}_i^2) + G \sum_{j < i} \frac{m_j}{|\mathbf{r}_{ij}|} \right) \quad (8)$$

and fixing the time, the transversality condition is

$$\sum_i m_i (\dot{r}_i dr_i^s + r_i^2 \dot{\theta}_i d\theta_i^s + r_i^2 \sin^2 \theta_i \dot{\phi}_i d\phi_i^s) = 0 \quad (9)$$

or more compactly

$$\mathbf{P} \cdot d\mathbf{r}^s = 0 \quad (10)$$

where \mathbf{P} is the total momentum and $d\mathbf{r}^s$ any vector in the end manifold, a general result constraining the end manifold. If the velocity action, expression (5), is used a modified form of the transversality condition applies:

$$\sum_i m_i (\dot{r}_i dr_i^s + r_i^2 \dot{\theta}_i d\theta_i^s + r_i^2 \sin^2 \theta_i \dot{\phi}_i d\phi_i^s) - \sum_i m_i \dot{r}_i dr_i^s - \sum_i m_i r_i \dot{r}_i dr_i^s = 0. \quad (11)$$

If the end point under consideration has fixed angles and radial velocities, the left hand side of equation (11) vanishes identically. The velocity-action transversality condition thus tells us nothing about the manifolds on which the end-points lie. At the same time, the velocity action imposes no additional restrictions on the end manifolds over the position action.

⁴See Appendix A for detailed formulae.

3. The Second Variation

We now come to the question of how far the minimization of the action integral can be used to reproduce the dynamic equations, that is, the limit of the least-action method strictly defined. The limit may be pictured geometrically by using *kinetic foci* as defined by Thompson and Tait (1896, section 357, p. 428)⁵: “If, from any one configuration, two courses differing infinitely little from one another have again a configuration in common, this second configuration will be called a kinetic focus relatively to the first: or (because of the reversibility of the motion) these two configurations will be called conjugate kinetic foci.” It can be shown (for instance, by Whittaker 1959, pp. 251-3) that the action is neither a maximum nor a minimum over a path which includes a pair of kinetic foci.

More intuitively, if two paths infinitesimally close to each other between the same pair of end points both satisfy the Euler-Lagrange equations, the action (along either path) can no longer be a minimum (and the variation of the variation between them must vanish).

It is easiest to picture kinetic foci using a toy dynamical problem, that of finding the motion of a ball rolling on a large sphere, without friction or other complicating effects. Geodesics on the spherical surface are paths of least action in this case. Clearly there is a unique minimum path for points close together; that is, if two end points are chosen near each other, a portion of the great circle joining them gives the least action. As the points are taken farther and farther apart the action increases while staying a minimum. When the points are taken to be opposite each other, however, there is an infinite number of solutions all of the same length. Dynamically, the ball leaves the starting point and follows a geodesic to the antipode; but if it had left the starting point at a slightly different angle, it would still pass through the same antipode. On a sphere, then, kinetic foci are exactly opposite each other.

Still considering the motion of the ball dynamically, if the trajectory is extended, worse happens. The path taken, which passes more than halfway around the sphere, is actually longer than paths which follow the complement of the great circle. In fact it is longer than some small circles.

Geodesics on a torus provide greater complexity. Given any two points on the torus there will be a global minimum; a local minimum path, going the other way around the major radius; and an infinite series of other local minima, wrapping around one leg or the other of the torus. None of these can be continuously varied into another because of the different number of wrappings. The action (the length of the geodesic) tends to infinity as the wrappings increase.

⁵Page and section numbers are identical in the 1962 Dover reprint.

A more mathematically rigorous and useful, but also more complicated, treatment of the second variation takes us into Morse Theory.

3.1. Morse Theory

Marston Morse (1934) conducted an extensive study of the general topological properties of variational problems and their solutions. A summary of some of his results is presented below⁶.

An *extremal* is a path which satisfies the Euler-Lagrange equations. A *critical* extremal is one which makes the action a minimum.

A function which will play a part in what follows is defined by

$$2\Omega(s_i, \dot{s}_i) = \frac{\partial^2 L}{\partial \dot{r}_i^2} \dot{s}_i^2 + 2 \frac{\partial^2 L}{\partial r_i \partial \dot{r}_i} s_i \dot{s}_i + \frac{\partial^2 L}{\partial \dot{r}_i^2} \dot{s}_i^2 \quad (12)$$

for some integrand L and functions $s_i(t)$. The *characteristic form* is⁷

$$Q(z, \lambda) = \int_{t_0}^{t_1} 2 (\Omega(s_i, \dot{s}_i) - \lambda s_i \dot{s}_i) dt. \quad (13)$$

For a given extremal with fixed end points, the *accessory boundary problem* is defined as

$$\frac{d}{dt} \left(\frac{\partial \Omega}{\partial \dot{s}_i} \right) - \frac{\partial \Omega}{\partial s_i} + \lambda s_i = 0. \quad (14)$$

A solution s_i to this equation not identically zero is an *eigensolution* (sometimes *eigenvector*) and λ an *eigenvalue*. The *index* of an eigenvalue is the number of linearly independent eigensolutions corresponding to the eigenvalue.

For free end points the characteristic form is

$$Q(z, \lambda) = \sum_{h,k} b_{hk} u_h u_k + \int_{t_0}^{t_1} 2 (\Omega(s_i, \dot{s}_i) - \lambda s_i \dot{s}_i) dt \quad (15)$$

where b_{hk} , u_h and u_k are derived from the second variation at the end points and are given in Appendix A. The accessory boundary problem, equation (14), stays the same in form but the solution s_i must now satisfy the transversality condition.

⁶A shorter and somewhat more accessible presentation of most of Morse's results is found in Milnor (1963).

⁷Here z is used as a shorthand symbol for the collection of functions s_i , and below it includes also u_h and u_k .

If the problem is to find the geodesic in a space of a given metric between two manifolds of some description, the coefficients b_{hk} are a measure of the curvature of the manifolds. In particular, when the coefficients vanish the manifolds are flat.

If $\lambda = 0$ the accessory boundary problem becomes the *Jacobi equation* (not to be confused with the Hamilton-Jacobi equation), which is identical to the perturbed Euler-Lagrange equation. If there exist two points on an extremal at which an eigensolution with eigenvalue zero vanishes, these points are *conjugate points*. A *non-degenerate* extremal is one which has no zero eigenvalues in the accessory boundary problem. It is easily shown that conjugate points (mathematically defined) and kinetic foci (dynamically defined) are identical.

Determining the least-action limit for a given variational problem is thus the same as determining the first zero of the Jacobi function (after the initial point). This determination is not generally an easy thing to do. To take a specific example, for a group of bodies moving under each other's gravity the Jacobi function \mathbf{s} satisfies

$$\ddot{\mathbf{s}}_i = G \sum_{j \neq i} m_j \left(\frac{3\mathbf{r}_{ij}\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|^5} - \frac{1}{|\mathbf{r}_{ij}|^3} \right) \cdot \mathbf{s}_i. \quad (16)$$

Clearly, solving this is not a convenient way of finding kinetic foci. Not only is this less amenable to integration than the original dynamic equation, but the original equation must be solved first (which makes the locating of kinetic foci as a step in solving the dynamical problem rather pointless). A more practical method for use in calculation is called for.

3.2. Choquard's Criterion

Choquard (1955) studied the motion of bodies in strongly anharmonic potentials in the context of a semi-classical treatment of Feynman integrals. He found that multiple solutions to a dynamical problem were possible through the action of "forces of reflection", which allowed indirect paths from one end point to the other. In an indirect path, which corresponds to a stationary rather than a minimum action, at some time between the end points

$$\begin{aligned} \frac{d}{dt}(T) &= 0 \\ &= \frac{d}{dt} \left(\frac{1}{2m} \mathbf{p}^2 \right) \\ &= \frac{1}{m} \mathbf{p} \cdot (-\nabla V). \end{aligned} \quad (17)$$

That is, the momentum must be normal to the force.

To make this reasoning directly applicable to the problem at hand, consider a solution to the dynamical equations with a given set of end points, $\mathbf{r}(t)$; it must conserve total

energy E , made up of a kinetic part T and a potential part V . A varied path $\mathbf{r}(t) + \mathbf{s}(t)$ (where $\mathbf{s}(t)$ is a Jacobi function) also conserves an energy $E + \delta E = T + \delta T + V + \delta V$, and thus the Jacobi function itself conserves $\delta T + \delta V$. Since V is a function only of \mathbf{r} , not $\dot{\mathbf{r}}$, δV is a function only of \mathbf{s} , and for $|\mathbf{s}|$ small (which it is by definition) a linear function. This means that δV reaches its extreme value when \mathbf{s} does, and at the same point δT has an extremum. Since $|\mathbf{s}|$ can vanish only after its maximum, this point of extremum must occur before a conjugate point. The extremum of δT is given by

$$\frac{d}{dt}(\delta T) = 0. \quad (18)$$

Writing kinetic energy in terms of momentum,

$$\begin{aligned} T + \delta T &= \frac{1}{2m} (\mathbf{p} + \delta \mathbf{p})^2 \\ \delta T &\simeq \frac{1}{m} \mathbf{p} \cdot \delta \mathbf{p} \\ &= \frac{1}{m} \mathbf{p} \cdot (-\nabla V) \delta t \end{aligned} \quad (19)$$

so the condition for an extremum of the variation in kinetic energy is

$$\begin{aligned} \frac{d}{dt}(\delta T) &= 0 \\ \frac{1}{m} \mathbf{p} \cdot (-\nabla V) &= 0 \end{aligned} \quad (20)$$

and Choquard's criterion is recovered. For a situation with multiple particles, the varied path \mathbf{s} may be taken to be different from zero for only one of the particles. This leads to the conclusion that *a conjugate point may occur only after the point where the momentum is normal to the force on some body in the system*. Keeping in mind the identity of conjugate points and kinetic foci as well as Whittaker's result (above), Choquard's criterion gives a lower bound to the applicability of the least-action calculation. Following the trajectory of a dynamic system from the initial point, it is a minimum of the action at least until the momentum of some body is normal to the force on that body. This provides some insight into the shape of stationary-solution trajectories, as well as (with a further result of Morse, below) allowing a conclusion to be drawn as to the total number of solutions of all kinds⁸.

3.3. More Morse

There are several more results from Morse (1934) which are of use in the present problem. First we require a few more definitions:

⁸Choquard (1955) notes that his criterion does not apply to situations in which the trajectory is *always* normal to the acceleration, as in (for example) circular motion. However, these situations are generally symmetrical enough to allow the useful application of Jacobi functions.

A *Riemannian* space possesses a positive-definite metric which can be expressed as a quadratic form:

$$ds^2 = \sum_{i,j} g_{ij} dx^i dx^j. \quad (21)$$

The *connectivity* P_k of a space⁹ is the number of distinct homologous families of figures of dimension $k + 1$; that is, within each family one figure can be transformed into another by a continuous transformation, but a figure in one family cannot be so transformed into a figure in another. On a sphere, for instance, the connectivity P_0 is one, since any line may be transformed into another by a continuous transformation. On a torus P_0 is infinite, since there is an infinite number of families of curves distinguished from each other by the number of times they wrap about the large or small radii.

Morse is concerned with the connectivities of the *functional domain* Ω of admissible curves for a given variational problem¹⁰, that is those curves which have the required end points and are continuous along with their first derivatives. For the case of a set of trajectories in three dimensional space it is easiest to consider them transformed into a single trajectory in $3n$ -dimensional space, between two end points representing the starting and ending configurations. Each point in Ω represents a trajectory in the $3n$ -dimensional space. Since no points in $3n$ -space are excluded, any trajectory can be continuously transformed into any other; so any point in Ω can be continuously transformed into any other. Any line in Ω can then be transformed point by point into any other line, any plane figure likewise, and so on for all dimensions. Consequently each connectivity of the space of trajectories is one.

Morse's important results are:

An extremal which affords a minimum has no negative eigenvalues in the associated boundary problem. This is equivalent to saying it contains no conjugate points. Further, *the number of conjugate points of an end point of an extremal g on g is equal to the number of negative eigenvalues in the associated boundary problem.*

The index of an extremal is the sum of the indices of the conjugate points of an end point on the extremal.

The conjugate points of an end point of an extremal g on g form a set of measure zero. This means they are isolated (and thus much easier to deal with). More importantly, it means that the probability of choosing a pair of conjugate points by chance when setting up the variational problem is essentially zero.

⁹This is not to be confused with the *connection* of a space, or whether a space is *simply connected* (themselves distinct topological concepts).

¹⁰This is *not* the function $\Omega(s, \dot{s})$ found above and in Appendix A. The ambiguity in notation is regretted, but it should not lead to confusion.

If for a given Riemannian space R and terminal manifold Z there exists an integral I defined on R such that all critical extremals are non-degenerate, then the number of distinct extremals of index k is greater than or equal to the connectivity P_k of the functional domain Ω . If the extremals are of increasing type, the number of extremals of index k is equal to the connectivity P_k .

The last is a most useful result. However, to apply it we must show that the variational problem meets the requirements.

As demonstrated for example by Whittaker (1959, pp. 247-8, 254)¹¹ the dynamic equations of a system which has an integral of energy E can be derived by requiring that the variation of the integral

$$\int 2T dt \tag{22}$$

(where T is the kinetic energy) vanish, for a fixed value of E . This formulation is known as Euler's Principle. For a system in which the total energy E is the sum of the kinetic energy T (quadratic in velocities) and potential energy V , the integral (22) can also be written as

$$\begin{aligned} I &= \int 2(E - V)^{1/2} (T)^{1/2} dt \\ &= \int 2(E - V)^{1/2} (a_{ij} \dot{x}^i \dot{x}^j)^{1/2} dt. \end{aligned} \tag{23}$$

This is the integral giving arc length on a surface of metric

$$g_{ij} = 4(E - V) a_{ij} \tag{24}$$

and the space of the possible solutions to our variational problem when formulated this way is indeed Riemannian, with geodesics corresponding to variational solutions. The cosmological variational problem in proper coordinates can be put into this form, so Morse's results apply. Further, the integral is of increasing type (since kinetic energy is always positive), so the number of solutions is given definitely.

Unfortunately, Morse's result cannot be applied directly to Hamilton's principle, as the functional domain is not Riemannian. The Lagrangian cannot be put in the necessary form of expression (23), since the potential energy forms a separate term which is not quadratic in the velocity differentials. This means that, if the preceding theory is to be used, either the problem must be put in Euler's form or some connection of a topological nature must be made between the two Least Action principles. The latter is addressed in the next section.

Before leaving Morse Theory, however, it is worthwhile to note the effect of the end manifolds of the velocity action on the number of solutions. Comparing the characteristic forms and accessory boundary problems between fixed-point and manifold situations, we

¹¹See also Arnold (1989), pp. 245ff.

find that the difference lies in the transversality condition and the quantities $b_{hk}u_hu_k$. It has already been shown that, using Euler's Principle, the transversality condition holds identically.

For an initial configuration manifold and Hamilton's Principle, combining two formulae from Appendix A,

$$\begin{aligned}
b_{hk}u_hu_k &= \left[\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) \frac{d^2 t^s}{de^2} + \left(\frac{\partial L}{\partial t} - \sum_i \frac{\partial \dot{q}_i}{\partial t} \frac{\partial L}{\partial \dot{q}_i} \right) \left(\frac{dt^s}{de} \right)^2 \right. \\
&\quad \left. + 2 \sum_i \left(\frac{\partial L}{\partial \dot{q}_i} \frac{dt^s}{de} \frac{d\dot{q}_i^s}{de} + \frac{\partial L}{\partial \dot{q}_i} \frac{d^2 \dot{q}_i^s}{de^2} \right) \right]_1 \\
&= \sum_i m_i \left(\dot{r}_i \frac{d^2 r_i^s}{de^2} + r_i^2 \dot{\theta}_i \frac{d^2 \theta_i^s}{de^2} + r_i^2 \sin^2 \theta_i \dot{\phi}_i \frac{d^2 \phi_i^s}{de^2} \right). \tag{25}
\end{aligned}$$

Comparing this with equations (9) and (10) the manifold curvature expression $b_{hk}u_hu_k$ is seen to be the dot product of the total momentum vector with a vector in the end-manifold surface:

$$b_{hk}u_hu_k = \mathbf{P} \cdot \frac{d^2}{de^2} \mathbf{x}^s \tag{26}$$

which is, near an extremal,

$$b_{hk}u_hu_k = \mathbf{P} \cdot \Delta \mathbf{x}^s / e^2. \tag{27}$$

For an extremal, the transversality condition requires that $\mathbf{P} \cdot \Delta \mathbf{x}^s = 0$ (see equation 10). More generally, since \mathbf{P} is a constant of motion belonging to the solution (not related to any particular variation around it) and e and $\Delta \mathbf{x}^s$ are independently arbitrary, $\mathbf{P} \cdot \Delta \mathbf{x}^s$ cannot vary with e , and thus must vanish (unless $b_{hk}u_hu_k$ is allowed to be infinite, a pathological case I propose to ignore). The dot product vanishing causes $b_{hk}u_hu_k$ to vanish as well. The same result holds if Euler's Principle is used.

For the velocity action and the final end manifold, with angles and radial velocities fixed, $b_{hk}u_hu_k$ vanishes identically using either Least Action Principle. Thus for each case *the fact that the ends of the action integral lie on manifolds and not on fixed points is irrelevant to the number of solutions*. Interpreted geometrically, the manifolds are flat surfaces.

4. The Number of Solutions

4.1. Catastrophe Theory

Applying Morse's result on the number of solutions to the problem formulated using Euler's Principle (which is the only way it is directly applicable), we find that there is one minimal extremal, plus one non-minimal extremal for each integral number of conjugate points. There are values of total energy for which there are no solutions. Most obvious

are those below the potential energy of the final end point; those are excluded from the functional domain at the outset. For values of the total energy in a gravitational system which are positive, especially strongly so, there can be only one solution since the Jacobi function for a nearly straight-line trajectory never returns to zero; the saddle-point solutions for these situations can be thought of as occurring at infinite values of total time.

But the calculation contemplated (and as performed by Peebles and those following his technique) uses Hamilton's Principle. To apply Morse to Hamilton a connection must be made between them. This can be done by way of the dynamical equations and Catastrophe Theory.

Consider a two-dimensional slice of the functional domain Ω , the dimensions being the Eulerian action (time integral of the kinetic energy T) and the Hamiltonian action (time integral of the Lagrangian function $T - V$). Choose the slice so that it contains all the extremals of the problem (see Figure 1). A given value of total energy will plot as a curve in this slice, with a minimum of $\int T dt$ at the location of the least-action trajectory and other extremals spaced along it (the latter may show as maxima, minima or points of inflection in this plot). Since the integrand of Euler's Principle is positive-definite, the least-action solution takes the minimum time of all the solutions for a given energy; the saddle-point solutions take increasing amounts of time for increasing index. All solutions will be equilibrium points for the potential represented by the action. The slice is thus a Poincaré diagram to which Catastrophe Theory applies, with total energy as the control parameter. The minimum solutions correspond to stable equilibria, the saddle-points to unstable equilibria.

In the same slice plot curves of constant total time. The index of a given extremal depends only on the number of kinetic foci of the trajectory, not on the action principle (if any) used to calculate it; in addition, all extremals are solutions to the dynamic equations. Thus the minimum of $\int L dt$ for each time corresponds to a minimum of $\int T dt$ for fixed total energy, and the non-minimum extremals will similarly correspond to non-minimum extremals of the Eulerian action for other values of total energy. Again, we have constructed a Poincaré diagram (rotated 90° with respect to the first), with total time as the control parameter.

There is at least one least-action solution for a given value of time. If there were two (or more), the chain of Eulerian least-action solutions would have a maximum or a minimum in total time, as shown in Figure 1. There are several reasons why this cannot happen; two are outlined below.

First, viewed as a Poincaré diagram in Hamiltonian extremals, Figure 1 requires two chains of *similar* (stable or unstable) equilibria to meet. This sort of topology, a bifurcation without an exchange of stability, is forbidden by Catastrophe Theory; therefore there is only one least-action Hamiltonian extremal. Similarly, there can only

be one saddle-point Hamiltonian extremal for each saddle-point Eulerian extremal¹².

Second, note that at a bifurcation point (point C in figure 1)

$$\left| \frac{\partial^2 I}{\partial q_i \partial q_j} \right| = 0 \quad (28)$$

for the action I and variables q in the two-dimensional slice; but this is just the requirement for a degenerate extremal, to which Morse's results specifically do not apply. Since, as noted above, these require some special symmetry in the problem and are almost impossible to generate by chance, it is reasonable to assume that our problem does not have them¹³.

We are finally in a position to determine how many solutions there are to the cosmological variational problem.

If the question is posed in a strictly proper-coordinate, Newtonian manner it comes out something like this: given a number of bodies moving under the influence of each other's gravity, all constrained to occupy the same position at time zero, and having given positions (or positions in two dimensions, radial velocities in the third) now; how many possible trajectories are there?

If the problem is formulated using the Eulerian action (minimum kinetic energy for fixed total energy), the space of solutions is Riemannian and the extremals are of increasing type. There is thus one minimum (and one stationary solution for each number of kinetic foci). By way of Catastrophe Theory this is connected to the Hamiltonian action (the form in which the question is asked above), which excludes some solutions which require a different value of total time. *There is one minimum solution and a finite number of stationary solutions.*

For small values of total time the energy will be forced to be positive (in order for the system to get from one configuration to the other, the speeds must be large, hence the kinetic energy large and positive) and only the least action solution will appear. This idea will be expanded below.

Note that if there is no integral of energy these results do not apply. Thus if a calculation attempts to compute the trajectories of a number of galaxies in

¹²Expositions of Catastrophe Theory are found in Lamb (1932, sect. 377, pp. 710-12) and Jeans (1919, sect. 18-23, pp. 20-6); the detailed demonstration of the necessity of an exchange of stability is found in Poincaré (1885).

¹³It might be possible to exclude them explicitly from the functional domain Ω , avoiding any problems at the start. However, it is conceivable that such an exclusion would change the topology of Ω and thus complicate the question of the connectivities of the space. For present purposes it is easier to deny them any place in the problem at the end.

a time-dependent, external tidal field, or any other case in which only part of an interacting system is modelled, the number of solutions cannot be determined from this development¹⁴.

5. A Dynamical Example

The simplest useful example of a dynamical system in astronomy is the two-body problem, dealing with a pair of bodies of reduced mass M in an orbit of total energy E and angular momentum J . Imposing a spherical coordinate system (r, θ, ϕ) with the orbit in the plane of the equator ($\theta = \pi/2$), the trajectory is given by

$$r = \frac{R_0}{1 + e \cos \phi} \quad (29)$$

with e the eccentricity of the orbit and $R_0 = J^2/GM$. Defining the Jacobi functions in each of the coordinates as $\delta r = s$, $\delta \theta = \xi$, $\delta \phi = \eta$ and the perturbations in energy and angular momentum as h and l respectively, one eventually finds

$$\xi = \xi_0 \sin(\phi - \phi_0) \quad (30)$$

$$\frac{d\eta}{d\phi} = \frac{l}{J} - 2\frac{s}{r} \quad (31)$$

$$\begin{aligned} \text{for } e < 1, s = & \frac{hGM}{2E^2} \left[F \sin \phi + e + \left(\frac{El}{Jh} \frac{e^2 - 1}{e} - \frac{e^2 + 1}{2} \right) \cos \phi \right. \\ & \left. - \frac{1}{2} \frac{e \sin^2 \phi}{1 + e \cos \phi} - \frac{3e^2}{\sqrt{1 - e^2}} \sin \phi \arctan \left(\frac{\sqrt{1 - e^2}}{1 + e} \tan \frac{\phi}{2} \right) \right] \end{aligned} \quad (32)$$

$$\begin{aligned} \text{for } e > 1, s = & \frac{hGM}{2E^2} \left[F \sin \phi + e + \left(\frac{El}{Jh} \frac{e^2 - 1}{e} - \frac{e^2 + 1}{2} \right) \cos \phi \right. \\ & \left. - \frac{1}{2} \frac{e \sin^2 \phi}{1 + e \cos \phi} - \frac{3e^2}{2\sqrt{e^2 - 1}} \sin \phi \ln \left| \frac{\sqrt{e^2 - 1} \tan(\phi/2) + 1 + e}{\sqrt{e^2 - 1} \tan(\phi/2) - 1 - e} \right| \right] \end{aligned} \quad (33)$$

where F is a constant used to adjust the zero point of s . The first expression for s is used for bound (elliptical) orbits, the second for unbound (hyperbolic). The practical difficulty of calculations using Jacobi functions is evident.

¹⁴This does not mean that Layzer's (1963) cosmic energy equation exempts all interesting distributions of astronomical objects from the results obtained here. An integral of energy still exists for any collection of masses interacting through gravity; Layzer's equation only states that a quantity based on comoving motions and coordinates, which resembles Newtonian energy in some respects, is not conserved. Since the number of solutions a problem has should not depend on which particular variables are used to write it down, results obtained herein using proper, inertial coordinates apply also to calculations performed in other ways.

The out-of-plane Jacobi function ξ is, however, simple and gratifyingly general. For any eccentricity (indeed, even for unbound trajectories) conjugate points are found on diametrically opposite sides of the orbit. This is easy to picture: rotation of the orbit through an infinitesimal (or even larger) angle around a line from the orbiting body through the primary, certainly an allowed variation, leaves the opposite point unchanged.

For very small e , that is for orbits close to circular, s becomes a simple sine function also, returning to zero after half an orbit. For $e \sim 1$, that is for orbits close to a parabola, analysis is a bit more complicated, though s is approximately sinusoidal and in no case does s reach zero again until after half an orbit. For $e > 1$, but not by much, s remains approximately sinusoidal. For very large e the approximation is better, that is the points where s vanishes are closer to being 180° in longitude away from each other; but the (unbound) trajectory might not include enough movement in longitude to provide a conjugate point for some initial points.

The Jacobi function in longitude, η , has a behavior which is in full even more complicated. However, note that its derivative is directly related to s . It can therefore not return to zero until well after s changes sign. Among the three Jacobi functions, then, ξ has its first zero after exactly half an orbit, while the other two take longer; so *The earliest zero for any perturbation in a two-body system occurs after half an orbit, so kinetic foci are 180° apart.*

Choquard's criterion is much easier to apply. There are two points where the momentum is normal to the gradient of the potential, at pericenter and apocenter; any pair of conjugate points must lie on opposite sides of one of these. Together with Morse's count of solutions to the Eulerian variational problem this means that there is an infinite number of solutions for a given set of end points, one for each half-integral number of revolutions of the orbit. As noted above, trajectories with energy lower than the lower of the potential energies of the end points are excluded from consideration. Those with positive energy have one least-action solution and possibly one saddle-point solution at finite times (depending on whether the first end point is taken far enough away from perihelion to allow the kinetic focus, 180° away in longitude, to appear on the trajectory); the rest at infinite times.

Applied to systems with many bodies, saddle-point solutions correspond to some sort of multiple-pass trajectory. If there are two bodies in an orbit that approximates isolated two-body motion, they can generate kinetic foci for the whole system.

Given a bound two-body system with a set of endpoints and a fixed time taken to go between them, the minimum-action solution will give a trajectory made up of less than half an orbit. The first stationary-action solution will contain more than half an orbit, a longer distance, which means a higher speed and thus higher kinetic energy. The second stationary solution will require at least three times the speed of the minimum solution, thus nine times the kinetic energy; few such orbits are bound. The situation

for a many-body system is rather more complicated, but for most astronomical systems a significant increase in the kinetic energy will make total energy positive and thus the system will become unbound. In this way the relatively small binding energy of astronomical systems severely limits the number of saddle-point solutions (unless there is, say, one or more tightly orbiting pairs of objects).

6. Continuum Solutions

The discrete body approach to galaxy dynamics is of course an approximation. It may be justified by the fact that present distances between galaxies are significantly larger than galaxy dimensions, or (more practically) on the basis of our ignorance of their detailed mass distributions (including such things as dark matter halos). But if we are to consider the motions of galaxies all the way back to their formation it becomes an increasingly bad approximation, and it would be better to consider a continuous fluid of gravitating matter.

Indeed, the present picture of galaxy formation has them condensing out of a smooth fluid. It would be highly desirable to be able to follow this process in detail while requiring a certain configuration as a final end point. One could investigate, for example, the importance of mergers in galaxy dynamics, as well as the problems encountered by Dunn and Laflamme (1995) in matching a least-action calculation to an n-body simulation.

However, in attempting this we are faced with a massive theoretical complication as the number of degrees of freedom goes from $3n$ to infinite¹⁵. Additional practical difficulty is involved with the increased complexity of the calculation, using three equations (continuity, Euler's and Poisson's) instead of one. However, it can be done, as Susperreggi and Binney (1994) have shown (though it tends to be computationally intensive).

Consider, as a first approximation to a continuous-fluid situation, a large N-body calculation. Since the results of Morse Theory do not depend on the number of bodies, there still remains one minimum action solution and a finite number of stationary action solutions. (The bodies are now of all the same mass, and are labelled with, say, their ending coordinates instead of "M31"; but the Morse-based results are unchanged.) Adding more bodies increases the resolution of the simulation and the computational burden, but does nothing to the theory of solutions. Therefore, so far as a continuous fluid may be considered as made up of discrete masses, however tiny, there remains one least-action solution and one stationary solution for each possible value of the index.

¹⁵This is of less practical importance, as a continuum calculation always has some sort of short-wavelength cutoff (which is addressed in more detail below).

6.1. Orbit-Crossing and Kinetic Foci

Giavalisco et al. (1993) identified orbit-crossing as a major cause of multiple solutions, that is, when trajectories from different parts of the fluid occupy the same point at the same time. This makes the mapping of velocity to distance (a major concern of observational cosmology) multiple-valued. However, our question—the number of ways the present velocity and density distribution can arise from the Big Bang—is different, and orbit-crossing is not necessarily relevant.

To see this, consider a spherically symmetric part of a nearly uniform universe, of critical density for definiteness. Suppose that a small perturbation makes one shell slightly more dense than average and the shell contained immediately within it less dense. Over time the dense shell will expand at a slower rate than the universe as a whole, and the less dense shell faster; eventually their trajectories will meet, and there will be orbit-crossing (even with all shells expanding).

To locate the kinetic foci, first write the dynamical equation of a shell which contains a mass $m(r)$ within a radius r :

$$\ddot{r} = -\frac{Gm(r)}{r^2} \quad (34)$$

which has the Jacobi equation

$$\ddot{s} = \frac{2Gm(r)}{r^3}s \quad (35)$$

which, for shells near critical density, becomes

$$\ddot{s} = \frac{1}{9t^2}s. \quad (36)$$

In any spherically symmetric case s can start from zero and go back to zero only after r changes sign. In a critical universe (and, indeed, in any universe before a Big Crunch) this never happens; thus there are no kinetic foci. *Orbit-crossing does not necessarily generate kinetic foci.*

Now consider another nearly uniform universe, but this time allow several mass condensations to form. Place them in such a way as to generate two binary systems, and allow the tidal torque of each on the other to send them into bound orbits. In all this allow none of the trajectories of mass elements to cross. After half an orbit kinetic foci will be generated. *Kinetic foci do not necessarily generate orbit-crossing.*

Certainly an orbit-crossing situation in the context of the cosmological problem demands that two mass elements start in the same place (where all mass elements start, the origin) and end in the same place (where their trajectories cross). At first glance this appears to involve two trajectories with identical (proper space) endpoints, and thus two solutions to the equations of motion. But a solution is made up of all the trajectories of the bodies included, and whether it is a saddle-point or a minimum is an attribute of the solution as a whole, not of any of these bodies. In fact the two bodies that share end

points in an orbit-crossing situation are two solutions to slightly different equations of motion, not two different solutions to the same equation.

6.2. Potential Flow and Kinetic Foci

A useful simplification, then, for a continuum least-action calculation would be one that eliminates closed orbits; that is, one in which there is no rotation. Susperreggi and Binney (1994) used a velocity field derived from a potential suggested by Herivel (1955):

$$\mathbf{v}(x, y, z, t) = \nabla\alpha(x, y, z, t). \quad (37)$$

The field thus derived is both laminar and irrotational; the first term refers to the fact that it can have no orbit-crossing, and the second to the fact that it can have no vorticity:

$$\nabla \times \mathbf{v} = 0 \quad (38)$$

so they appear to have satisfied all parties.

Unfortunately, it is possible to have rotation in a flow that has no vorticity. Equation (38) is satisfied by a velocity field whose longitudinal (ϕ) component varies inversely with radius, $v_\phi \propto R^{-1}$; Lynden-Bell has pointed this out and, moreover, shows that it is just the sort of field one expects from tidal interactions (Lynden-Bell 1996). *A velocity field derived from a scalar potential can generate kinetic foci.*

6.3. Resolution and Kinetic Foci

The number of solutions in a continuum calculation thus formally remains the same, even if the restriction to potential flow is imposed: one minimum and one or several stationary solutions. Considering the latter the situation can appear rather depressing, since any two-body orbit by any pair of mass-elements, no matter how small, will generate kinetic foci and thus multiple solutions. It seems somehow unfair that a cosmological simulation should lose its minimum status through half the orbit of its smallest binary star. In practical terms, this means that a continuum least-action algorithm which is strictly minimizing will find only one solution, the one without so much as a half-orbit, which is not necessarily the right one; while an algorithm which finds all stationary solutions will find many possible answers, with no clue as to which is more probable.

But cosmological simulations rarely depict single stars. In practice there is always a scale below which no detail can be seen; kinetic foci on this scale cannot affect the minimum status of the calculation. In a very simple example, consider a triple star made up of one tight binary and one wide component. If all bodies are included, a solution will only be a minimum through half the orbital period of the close double. However if the

binary is modeled by a single mass, a solution will be a minimum through half the period of the wide component. It is a matter of choice which is the more important trajectory to calculate—or, alternatively, whether the computational burden of calculating several, perhaps many, stationary solutions is worth maintaining the higher resolution.

In a more complicated situation setting the desirable resolution is also more complicated. In a rich galaxy cluster, for instance, the dynamical timescale of the center regions is much shorter than the outskirts, and varies continuously with radius. What particular scale is best for the calculation? The answer is not obvious. However, the question is not restricted to least action calculations, so it is at least a familiar one.

7. Summary

The important results of this study are as follows:

If the action for the cosmological variational problem can be written in proper coordinates and an integral of energy exists, there is one minimum solution. Assuming Hamilton's Principle is used, there may be additional, stationary solutions, one for each number of kinetic foci, if multiple-pass trajectories exist. There is a finite number in total, limited by possible values of energy. Solutions containing at least one approximately two-body orbit which passes through more than 180° in longitude are not minima.

Kinetic foci are reached only after the momentum is normal to the force for some body in the system.

In so far as a continuous mass distribution may be approximated by an arbitrarily large number of individual masses, *a continuum least-action calculation also has a single minimum solution, but generally a very large number of stationary solutions.* These can be limited by setting a lower limit to the resolution of the calculation. The specific size of this resolution may be difficult to determine.

A radial velocity, rather than a distance, can be used as an end point in a numerical variational calculation. Forms of the modified action required have been discovered by Giavalisco et al. (1993) and used by Schmoldt & Saha (1998). *Using such an endpoint has no effect on the number or character of solutions.*

Orbit-crossing is not necessarily related to the number of solutions of a continuum calculation.

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A. Variable End Points

The following derivations follow Morse (1934) with some changes in notation and terminology. Courant and Hilbert (1953) have a derivation for the transversality condition which in fact results in the same formula; however, they require some assumptions about the end manifold which do not hold in the present situation.

A.1. The Transversality Condition

Suppose the problem to be that of minimizing the integral

$$I = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t) dt \quad (\text{A1})$$

subject to the condition that one or both of the end points are not fixed but must lie on end manifolds of some description. The solution to the problem is given by some extremal $g = g(t)$. Admissible curves for the problem will be those with end points near those of g and which are continuous along with their first and second derivatives. These curves are described by the r functions $\alpha_h(e)$ such that $\alpha_h(0)$ gives g . The end points in particular are given by

$$\begin{aligned} t^s &= t^s(\alpha_1, \dots, \alpha_r) \\ q_i^s &= q_i^s(\alpha_1, \dots, \alpha_r) \\ s &\in (1, 2) \end{aligned}$$

(the superscript 1 or 2 refers to the initial or final end point). Observe

$$q_i^s(\alpha_h(e)) = q_i^s(t^s(\alpha_h(e)), e) \quad (\text{A2})$$

where h takes on the values 1 to r .

Integral (A1) is now a function of e ; considered this way, the first variation (by Liebnitz' Rule) is

$$I'(e) = \left[L(t^s) \frac{dt^s}{de} \right]_1^2 + \int_{t_1(e)}^{t_2(e)} \sum_i \left(\frac{\partial L}{\partial q_i} \frac{\partial q_i}{\partial e} + \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial e} \right) dt. \quad (\text{A3})$$

After integration by parts and a bit of algebra, one obtains the Euler-Lagrange equations and

$$\left[\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) \frac{dt^s}{de} + \sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{dq_i^s}{de} \right]_1^2 = 0. \quad (\text{A4})$$

Again, the parametrization by e is arbitrary. If de is multiplied out of the above equation, the normal form of the *transversality condition* is obtained. If the manifold on which the end point is allowed to vary is specified by means of the differentials dq_i^s and dt^s , (A4) contains a condition fulfilled by the true minimizing end point. Conversely, the transversality condition can sometimes be used to gain some insight into the end manifold when only the Lagrangian and the fact of minimization are given.

If the integral to be varied is changed from (A1) to the velocity action,

$$\begin{aligned} I^* &= \int_{t_1}^{t_2} \left(L(q_i, \dot{q}_i, t) - \sum_j \frac{d}{dt} \left(q_j \frac{\partial L}{\partial \dot{q}_j} \right) \right) dt \\ &= I - \left[\sum_j q_j \frac{\partial L}{\partial \dot{q}_j} \right]_1^2 \end{aligned} \quad (\text{A5})$$

where j denotes those coordinates in which velocity rather than coordinate is fixed at the end point, the variation of the boundary term must be included in the transversality condition. A similar derivation to the above results in the *velocity-action transversality condition*:

$$\begin{aligned} &\left[\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - \sum_j q_j \frac{\partial^2 L}{\partial t \partial \dot{q}_j} \right) \frac{dt^s}{de} + \sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{dq_i^s}{de} \right. \\ &\quad \left. - \sum_j \left(\frac{\partial L}{\partial \dot{q}_j} + q_j \frac{\partial^2 L}{\partial q_j \partial \dot{q}_j} \right) \frac{dq_j^s}{de} - \sum_j q_j \frac{\partial^2 L}{\partial \dot{q}_j^2} \frac{d\dot{q}_j}{de} \right]_1^2 = 0. \end{aligned} \quad (\text{A6})$$

A.2. The Second Variation

Applying Liebnitz' Rule again gives

$$\begin{aligned} I''(e) &= \int_{t_1(e)}^{t_2(e)} \frac{\partial}{\partial e} \sum_i \left(\frac{\partial L}{\partial q_i} \frac{\partial q_i}{\partial e} + \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial e} \right) dt \\ &\quad + \left[\sum_i \left(\frac{\partial L}{\partial q_i} \frac{\partial q_i}{\partial e} + \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial e} \right) \frac{dt^s}{de} \right]_1^2 \\ &\quad + \left[\frac{\partial}{\partial e} (L(t^s)) \frac{dt^s}{de} \right]_1^2 + \left[L \frac{d^2 t^s}{de^2} \right]_1^2. \end{aligned} \quad (\text{A7})$$

After some algebra this becomes

$$I''(e) = \int_{t_1(e)}^{t_2(e)} \sum_i 2\Omega \left(\frac{\partial q_i}{\partial e}, \frac{\partial \dot{q}_i}{\partial e} \right) dt + \int_{t_1(e)}^{t_2(e)} \sum_i \frac{\partial^2 q_i}{\partial e^2} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \right) dt$$

$$\begin{aligned}
& + \left[\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) \frac{d^2 t^s}{de^2} + \left(\frac{\partial L}{\partial t} - \sum_i \frac{\partial \dot{q}_i}{\partial t} \frac{\partial L}{\partial q_i} \right) \left(\frac{dt^s}{de} \right)^2 \right. \\
& + \left. 2 \sum_i \left(\frac{\partial L}{\partial q_i} \frac{dt^s}{de} \frac{dq_i^s}{de} + \frac{\partial L}{\partial \dot{q}_i} \frac{d^2 q_i^s}{de^2} \right) \right]_1. \tag{A8}
\end{aligned}$$

The second integral vanishes for extremals.

While this version of the second variation is useful, it may be made a manifestly symmetric quadratic form in the variations

$$u_h = \frac{d\alpha_h}{de}. \tag{A9}$$

Using these in equation (A8) there results

$$\begin{aligned}
I''(e) &= \sum_{h,k} \left[\left(L - \sum_i \frac{\partial q_i}{\partial t} \frac{\partial L}{\partial \dot{q}_i} \right) \frac{\partial^2 t^s}{\partial \alpha_h \partial \alpha_k} + \left(\frac{\partial L}{\partial t} - \sum_i \dot{q}_i \frac{\partial L}{\partial q_i} \right) \frac{\partial t^s}{\partial \alpha_h} \frac{\partial t^s}{\partial \alpha_k} \right. \\
&+ \left. \sum_i \frac{\partial L}{\partial q_i} \left(\frac{\partial t^s}{\partial \alpha_h} \frac{\partial q_i^s}{\partial \alpha_k} + \frac{\partial t^s}{\partial \alpha_k} \frac{\partial q_i^s}{\partial \alpha_h} \right) + \sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{\partial^2 q_i^s}{\partial \alpha_h \partial \alpha_k} \right]_1^2 u_h u_k \\
&+ \sum_h \left[\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) \frac{\partial t^s}{\partial \alpha_h} + \sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{\partial q_i^s}{\partial \alpha_h} \right]_1^2 \frac{\partial^2 \alpha_h}{\partial e^2} \\
&+ \int_{t_1(e)}^{t_2(e)} \sum_i 2\Omega \left(\frac{\partial q_i}{\partial e}, \frac{\partial \dot{q}_i}{\partial e} \right) dt \\
&+ \int_{t_1(e)}^{t_2(e)} \sum_i \frac{\partial^2 q_i}{\partial e^2} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \right) dt. \tag{A10}
\end{aligned}$$

For an extremal satisfying the transversality condition, the coefficients of $\partial^2 \alpha_h / \partial e^2$ as well as the last integral vanish; and we are left with the second variation integral, as in the case of fixed end points, and a symmetrical quadratic form in the variations at the end points. The variations at the end points and within the integral are related by

$$\begin{aligned}
\frac{\partial q_i}{\partial e} &= \sum_h \left[\frac{\partial q_i}{\partial \alpha_h} - \dot{q}_i \frac{\partial t}{\partial \alpha_h} \right] u_h \\
\frac{\partial \dot{q}_i}{\partial e} &= \sum_h \left[\frac{\partial \dot{q}_i}{\partial \alpha_h} - \ddot{q}_i \frac{\partial t}{\partial \alpha_h} \right] u_h \tag{A11}
\end{aligned}$$

where evaluation is carried out at the end points. Morse defines the quantities b_{hk} for an extremal satisfying the transversality condition via

$$I''(0) = \int_{t_1(e)}^{t_2(e)} \sum_i 2\Omega \left(\frac{\partial q_i}{\partial e}, \frac{\partial \dot{q}_i}{\partial e} \right) dt + \sum_{h,k} b_{hk} u_h u_k \tag{A12}$$

and uses this notation for his definitions of the index form.

If the velocity action is used, the second variation of the boundary term must be calculated and added to the expression above. Following the lines of the above derivation

one finds

$$\begin{aligned}
I^{*''}(e) = & \int_{t_1(e)}^{t_2(e)} \sum_i 2\Omega \left(\frac{\partial q_i}{\partial e}, \frac{\partial \dot{q}_i}{\partial e} \right) dt + \int_{t_1(e)}^{t_2(e)} \sum_i \frac{\partial^2 q_i}{\partial e^2} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \right) dt \\
& + \left[\left(L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - \sum_j q_j \frac{\partial^2 L}{\partial t \partial \dot{q}_j} \right) \frac{d^2 t^s}{de^2} + \left(\frac{\partial L}{\partial t} - \sum_i \frac{\partial \dot{q}_i}{\partial t} \frac{\partial L}{\partial q_i} - \sum_j q_j \frac{\partial^3 L}{\partial t^2 \partial \dot{q}_j} \right) \left(\frac{dt^s}{de} \right)^2 \right. \\
& + 2 \sum_i \left(\frac{\partial L}{\partial q_i} \frac{dt^s}{de} \frac{dq_i^s}{de} + \frac{\partial L}{\partial \dot{q}_i} \frac{d^2 q_i^s}{de^2} \right) - \sum_j 2 \left(\frac{\partial^2 L}{\partial t \partial \dot{q}_j} + q_j \frac{\partial^3 L}{\partial t \partial q_j \partial \dot{q}_j} \right) \frac{dq_j}{de} \frac{dt^s}{de} - \\
& - \sum_j \left(\frac{\partial L}{\partial \dot{q}_j} + q_j \frac{\partial^2 L}{\partial q_j \partial \dot{q}_j} \right) \frac{d^2 q_j^s}{de^2} - \sum_j q_j \frac{\partial^2 L}{\partial \dot{q}_j^2} \frac{d^2 \dot{q}_j^s}{de^2} - \sum_j q_j \frac{\partial^3 L}{\partial \dot{q}_j^3} \left(\frac{d\dot{q}_j^s}{de} \right)^2 \\
& - \sum_j \left(2 \frac{\partial^2 L}{\partial q_j \partial \dot{q}_j} + q_j \frac{\partial^3 L}{\partial q_j^2 \partial \dot{q}_j} \right) \left(\frac{dq_j^s}{de} \right)^2 - \sum_j \left(2 \frac{\partial^2 L}{\partial \dot{q}_j^2} + q_j \frac{\partial^3 L}{\partial q_j \partial \dot{q}_j^2} \right) \frac{dq_j^s}{de} \frac{d\dot{q}_j^s}{de} \\
& \left. - \sum_j 2 \frac{\partial^3 L}{\partial t \partial \dot{q}_j^2} \frac{d\dot{q}_j^s}{de} \frac{dt^s}{de} \right]_1. \tag{A13}
\end{aligned}$$

Again, a symmetric form may be found for extremals which satisfy the transversality condition. Following the above derivation, one obtains

$$\begin{aligned}
I^{*''}(0) = & \sum_{h,k} \left[\left(L - \sum_i \frac{\partial q_i}{\partial t} \frac{\partial L}{\partial \dot{q}_i} - \sum_j q_j \frac{\partial^2 L}{\partial t \partial \dot{q}_j} \right) \frac{\partial^2 t^s}{\partial \alpha_h \partial \alpha_k} \right. \\
& + \left(\frac{\partial L}{\partial t} - \sum_i \dot{q}_i \frac{\partial L}{\partial q_i} - \sum_j q_j \frac{\partial^3 L}{\partial t^2 \partial \dot{q}_j} \right) \frac{\partial t^s}{\partial \alpha_h} \frac{\partial t^s}{\partial \alpha_k} \\
& + \sum_i \frac{\partial L}{\partial q_i} \left(\frac{\partial t^s}{\partial \alpha_h} \frac{\partial q_i^s}{\partial \alpha_k} + \frac{\partial t^s}{\partial \alpha_k} \frac{\partial q_i^s}{\partial \alpha_h} \right) + \sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{\partial^2 q_i^s}{\partial \alpha_h \partial \alpha_k} \\
& - \sum_j \left(\frac{\partial L}{\partial \dot{q}_j} + q_j \frac{\partial^2 L}{\partial q_j \partial \dot{q}_j} \right) \frac{\partial^2 q_j^s}{\partial \alpha_h \partial \alpha_k} - \sum_j q_j \frac{\partial^2 L}{\partial \dot{q}_j^2} \frac{\partial^2 \dot{q}_j^s}{\partial \alpha_h \partial \alpha_k} \\
& - \sum_j 2 \left(\frac{\partial^2 L}{\partial t \partial \dot{q}_j} + q_j \frac{\partial^3 L}{\partial t \partial q_j \partial \dot{q}_j} \right) \frac{\partial q_j^s}{\partial \alpha_h} \frac{\partial t^s}{\partial \alpha_k} - \sum_j q_j \frac{\partial^3 L}{\partial \dot{q}_j^3} \frac{\partial q_j^s}{\partial \alpha_h} \frac{\partial \dot{q}_j^s}{\partial \alpha_k} \\
& - \sum_j \left(\frac{\partial^2 L}{\partial q_j \partial \dot{q}_j} + q_j \frac{\partial^3 L}{\partial q_j^2 \partial \dot{q}_j} \right) \frac{\partial q_j^s}{\partial \alpha_h} \frac{\partial q_j^s}{\partial \alpha_k} - \sum_j \left(\frac{\partial^2 L}{\partial \dot{q}_j^2} + q_j \frac{\partial^3 L}{\partial q_j \partial \dot{q}_j^2} \right) \frac{\partial q_j^s}{\partial \alpha_h} \frac{\partial \dot{q}_j^s}{\partial \alpha_k} \\
& \left. - \sum_j 2 q_j \frac{\partial^3 L}{\partial t \partial \dot{q}_j^2} \frac{\partial \dot{q}_j^s}{\partial \alpha_h} \frac{\partial t^s}{\partial \alpha_k} \right]_1 u_h u_k \\
& + \int_{t_1}^{t_2} \sum_i 2\Omega \left(\frac{\partial q_i}{\partial e}, \frac{\partial \dot{q}_i}{\partial e} \right) dt \tag{A14}
\end{aligned}$$

$$= \sum_{h,k} b_{hk} u_h u_k + \int_{t_1}^{t_2} \sum_i 2\Omega \left(\frac{\partial q_i}{\partial e}, \frac{\partial \dot{q}_i}{\partial e} \right) dt. \tag{A15}$$

REFERENCES

- Arnold, V. I. 1989, *Mathematical Methods of Classical Mechanics*, 2nd. ed. (New York: Springer-Verlag, Inc.)
- Bondi, H. 1960, *Cosmology*, 2nd. ed. (Cambridge: Cambridge University Press); see especially chapter IX
- Choquard, P. 1955, *Helvetica Physica Acta*, 28, 89
- Courant, R., & Hilbert, D. 1953, *Methods of Mathematical Physics, Volume I* (London: Wiley-Interscience)
- Dunn, A. M., & Laflamme, R. 1995, *ApJ*, 443, L1
- Herivel, J. W. 1955, *Proceedings of the Cambridge Philosophical Society*, 51, 344
- Giavalisco, M., Mancinelli, B., Mancinelli, B. J. & Yahil, A. 1993, *ApJ*, 411, 9
- J Jeans, J. H. 1919, *Problems of Cosmogony and Stellar Dynamics* (Cambridge: Cambridge University Press)
- Lamb, H. 1932, *Hydrodynamics*, sixth edition (Cambridge: Cambridge University Press)
- Layzer, D. 1963, *ApJ*, 138, 174
- Lynden-Bell, D. 1996, *Current Science*, 70, 789
- Milnor, J. 1963, *Morse Theory* (Princeton: Princeton University Press)
- Morse, Marston 1934, *The Calculus of Variations in the Large* (New York: American Mathematical Society)
- Peebles, P. J. E. 1980, *The Large-Scale Structure of the Universe* (Princeton: Princeton University Press)
- Peebles, P. J. E. 1989, *ApJ*, 344, L53
- Peebles, P. J. E. 1990, *ApJ*, 362, 1

Peebles, P. J. E. 1994, ApJ, 429, 43

Poincaré, H. 1885, Acta Mathematica, VII, 259

Schmoldt, I. & Saha, P. 1998, AJ, 115, 2231

Susperregi, M., & Binney, J. 1994, MNRAS, 271, 719

Thompson, Sir William (Lord Kelvin), & Tait, P. G. 1896, A Treatise on Natural Philosophy, Volume 1 (Cambridge: Cambridge University Press); revised and published in 1912 as Principles of Mechanics and Dynamics, also by Cambridge University Press; the latter reprinted 1962 (New York: Dover).

Valtonen, M. J., Byrd, G. G., McCall, M. L., & Innanen, K. A. 1993, AJ, 105, 886

Whittaker, E. T. 1959, A Treatise on the Analytical Dynamics of Particles and Rigid Bodies, 4th edition (Cambridge: Cambridge University Press)

Fig. 1.— Poincaré diagram connecting the two Least Action Principles. For a given set of end points (or manifolds) a slice of the functional domain, which by construction contains all the solutions to the problem, is plotted. The Hamiltonian action is the vertical coordinate, the Eulerian action the horizontal coordinate. For a given value of total energy (the Eulerian control parameter; say, E_1 , E_2 or E_3) there will be a single minimum solution and a series of stationary solutions. For a given value of total time (the Hamiltonian control parameter, say t_1 , t_2 or t_3) there will be at least one minimum solution. In terms of Catastrophe Theory, the minimum solutions form a chain of stable equilibria (shown as a solid line in the figure), the stationary solutions a chain of unstable equilibria (not shown in this figure for clarity). If there were two Hamiltonian solutions on any Eulerian branch of solutions, as shown here, it would require the meeting of two chains of Hamiltonian similar equilibria (at point C) without an exchange of stability. Such a situation is forbidden by Catastrophe Theory, as described in the text.